

METHOD, SYSTEM, AND COMPUTER PROGRAM PRODUCT
FOR ANALYZING COMBINATORIAL LIBRARIES

ABSTRACT

The invention provides for *in silico* analysis of a virtual combinatorial library. Mapping coordinates for a training subset of products in the combinatorial library, and features of their building blocks, are obtained. A supervised machine learning approach is used to infer a mapping function f that transforms the building block features for each product in the training subset of products to the corresponding mapping coordinates for each product in the training subset of products. The mapping function f is then encoded in a computer readable medium. The mapping function f can be retrieved and used to generate mapping coordinates for any product in the combinatorial library from the building block features associated with the product.

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